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Molecular docking of medicinal plants: Towards metabolic disease management

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Abstract: The rising global burden of metabolic disease, together with the high cost and limited accessibility of conventional antidiabetic therapeutics in sub-Saharan Africa, has renewed interest in agriculturally cultivated medicinal plants as sustainable sources of bioactive phytochemicals with well-documented ethnopharmacological relevance. This study aimed to identify and prioritize phytochemicals with therapeutic potential against validated metabolic disease targets through an integrated computational drug discovery workflow. 14 bioactive phytochemicals from six agricultural medicinal plants- *Moringa oleifera*, *Vernonia amygdalina*, *Azadirachta indica*, *Curcuma longa*, *Hibiscus sabdariffa*, and *Zingiber officinale* were retrieved from PubChem and docked against five protein targets implicated in type 2 diabetes mellitus (T2DM) and metabolic syndrome: α-glucosidase (PDB: 3W37), dipeptidyl peptidase-4 (DPP-4; PDB: 2I78), peroxisome proliferator-activated receptor gamma (PPARγ; PDB: 2PRG), α-amylase (PDB: 1B2Y), and glucose transporter type 2 (GLUT2; PDB: 5EQG). Docking was performed in AutoDock Vina via PyRx 0.8, ADMET properties were predicted using SwissADME and ADMETlab 3.0, and a random forest classifier trained on ChEMBL 33 bioactivity data was used for artificial intelligence-assisted lead prioritization. Nimbolide from *A. indica* showed the strongest binding affinity, docking against PPARγ at - 8.4 kcal/mol, while hibiscetin from *H. sabdariffa* bound GLUT2 at - 7.6 kcal/mol. Quercetin and 6-gingerol inhibited α-glucosidase more strongly than the reference drug acarbose (- 6.5 kcal/mol). All priority leads satisfied Lipinski's Rule of Five and displayed favorable, low-risk ADMET profiles. The integration of ethnopharmacological plant selection, molecular docking, ADMET prediction, and AI-assisted prioritization identified nimbolide, hibiscetin, quercetin, and curcumin as promising, sustainable phytochemical leads for metabolic disease management in resource-limited settings.

Introduction

Metabolic disorders, including type 2 diabetes mellitus (T2DM), obesity, and dyslipidemia, constitute an escalating global public health burden [1]. The International Diabetes Federation estimates that 589 million adults aged 20 - 79 years were living with diabetes worldwide in 2024, corresponding to a global prevalence of 11.1% [1]. Although sub-Saharan Africa currently records the lowest regional prevalence (5.0%), the continent is projected to experience the largest proportional increase in disease burden, with an estimated 60 million cases anticipated by 2050; compounding this trajectory, up to 73.0% of diabetes cases across Africa remain undiagnosed [2]. The high cost, systemic adverse effects, and restricted availability of approved antidiabetic medications in low-resource settings have intensified interest in plant-derived therapeutic alternatives. Agriculturally cultivated species such as *Moringa oleifera* Lam. (Moringaceae), *Vernonia*

amygdalina Delile (Asteraceae), *Azadirachta indica* A. Juss. (Meliaceae), *Curcuma longa* L. (Zingiberaceae), *Hibiscus sabdariffa* L. (Malvaceae), and *Zingiber officinale* Roscoe (Zingiberaceae) are widely cultivated across West Africa and harbor diverse bioactive phytochemicals, including flavonoids (quercetin, hibiscetin, luteolin), terpenoids (nimbolide, vernodalin), phenolic acids (chlorogenic acid), diarylheptanoids (curcumin), and phenylpropanoids (6-gingerol). These constituents modulate glucose and lipid metabolism through multiple, and often complementary, molecular mechanisms [3-5]. Their dual role as staple food crops and reservoirs of bioactive metabolites positions them as particularly attractive candidates for sustainable drug discovery within Africa.

Advances in artificial intelligence (AI) and machine learning (ML) have considerably accelerated phytochemical drug discovery by enabling high-throughput analysis of large bioactivity datasets and probabilistic prediction of therapeutic activity [6, 7]. When combined with molecular docking and absorption, distribution, metabolism, excretion, and toxicity (ADMET) profiling, AI-driven workflows provide a cost-efficient means of preclinical screening for natural product libraries, without the resource demands of experimental bioassays [8-10]. The present study employed an integrated computational pipeline to identify and prioritize phytochemical leads acting on validated metabolic disease targets, evaluating their binding affinity, drug-likeness, and pharmacokinetic suitability, with a view to informing sustainable healthcare delivery across Africa.

Materials and methods

Ethnopharmacological plant selection: Six agriculturally cultivated medicinal plants- *M. oleifera*, *V. amygdalina*, *A. indica*, *C. longa*, *H. sabdariffa*, and *Z. officinale* with documented ethnopharmacological use in the management of metabolic disease across West Africa were selected following a systematic review of ethnobotanical literature, the NAPRALERT database, Dr. Duke's Phytochemical and Ethnobotanical Databases, and published Nigerian ethnomedicinal surveys. Selection criteria comprised: (i) established traditional use in the management of T2DM or related metabolic conditions; (ii) commercial cultivation or widespread distribution across sub-Saharan Africa; and (iii) availability of phytochemical data within open-access repositories.

Phytochemical and target protein retrieval: Three-dimensional structure data files (SDF) of 14 bioactive phytochemicals from the selected plants were retrieved from the PubChem Compound Database (https://pubchem.ncbi.nlm.nih.gov), with corresponding PubChem Compound Identifiers (CIDs) presented in **Table 1**. Structures were energy-minimized using the MMFF94 force field implemented in Open Babel (v3.1) to obtain geometrically optimized three-dimensional conformers. Target receptor proteins implicated in T2DM and metabolic syndrome pathogenesis were obtained from the RCSB Protein Data Bank (https://www.rcsb.org: α-glucosidase (PDB: 3W37), DPP-4 (PDB: 2I78), PPARγ (PDB: 2PRG), α-amylase (PDB: 1B2Y), and GLUT2 (PDB: 5EQG). Proteins were prepared in AutoDockTools (v1.5.7) by removal of co-crystallised water molecules, addition of polar hydrogens, and assignment of Gasteiger partial charges.

Molecular docking protocol: Molecular docking was performed using AutoDock Vina (v1.2) within the PyRx (v0.8) graphical interface [11]. Grid boxes were centered on the catalytic or ligand-binding site of each target protein, with a grid spacing of 0.375 Å and an exhaustiveness value of 32 to ensure comprehensive conformational sampling. Binding affinities were expressed in kcal/mol, with more negative values denoting stronger predicted ligand-receptor interactions. The reference antidiabetic agent acarbose was docked against α-glucosidase as a positive control for protocol validation. Post-docking visualization and interaction analysis were performed using BIOVIA Discovery Studio Visualizer (2024).

ADMET prediction: Absorption, distribution, metabolism, excretion, and toxicity properties of the prioritized leads were predicted using SwissADME (https://www.swissadme.ch) and ADMETlab 3.0 (https://admetlab3.

scbdd.com). Drug-likeness was evaluated against Lipinski's Rule of Five (molecular weight ≤ 500 Da, logP ≤ 5, hydrogen bond donors [HBD] ≤ 5, hydrogen bond acceptors [HBA] ≤ 10). Blood-brain barrier permeability, cytochrome P450 (CYP) inhibition profiles, and AMES mutagenicity predictions were additionally assessed.

AI-assisted lead prioritization: A random forest (RF) classification model, trained on ChEMBL 33 bioactivity data for T2DM-relevant targets (n = 14,872 compounds), was used to predict the probability of bioactivity (pActive) for each phytochemical. Molecular fingerprints (Morgan radius 2, 2048 bits), generated using RDKit, served as feature vectors. The model achieved a cross-validated accuracy of 84.6% and an area under the receiver operating characteristic curve (AUC-ROC) of 0.91. Compounds meeting a pActive threshold of ≥ 0.70 and a docking score ≤ - 6.5 kcal/mol were designated priority leads [10, 12].

Table 1: Bioactive phytochemicals for molecular docking, with corresponding PubChem CIDs and physicochemical descriptors

Plant species	Phytochemical	PubChem CID	MW (Da)	Molecular formula	Phytochemical class
Moringa oleifera	Quercetin	5280343	302.24	$C_{15}H_{10}O_7$	Flavonol
Moringa oleifera	Kaempferol	5280863	286.24	$C_{15}H_{10}O_6$	Flavonol
Moringa oleifera	Isothiocyanate [4-(α-L-rhamnosyloxy)benzyl]	9548634	369.42	$C_{13}H_{25}NO_9S$	Isothiocyanate
Vernonia amygdalina	Vernodalin	442495	314.29	$C_{17}H_{18}O_7$	Sesquiterpene lactone
Vernonia amygdalina	Luteolin	5280445	286.24	$C_{15}H_{10}O_6$	Flavone
Vernonia amygdalina	Chlorogenic acid	1794427	354.31	$C_{16}H_{18}O_9$	Hydroxycinnamic acid
Azadirachta indica	Nimbolide	12300180	466.52	$C_{27}H_{30}O_7$	Terpenoid lactone
Azadirachta indica	Azadirachtin	5281303	720.73	$C_{35}H_{44}O_{16}$	Limonoid tetranortriterpenoid
Curcuma longa	Curcumin	969516	368.38	$C_{21}H_{20}O_6$	Polyphenol/ diarylheptanoid
Curcuma longa	Bisdemethoxycurcumin	5315472	308.33	$C_{19}H_{16}O_4$	Diarylheptanoid
Hibiscus sabdariffa	Hibiscetin	5321879	318.24	$C_{15}H_{10}O_8$	Flavonol
Hibiscus sabdariffa	Delphinidin-3-glucoside	443650	465.37	$C_{21}H_{21}ClO_{12}$	Anthocyanin
Zingiber officinale	6-Gingerol	442495	294.39	$C_{17}H_{26}O_4$	Phenylpropanoid
Zingiber officinale	6-Shogaol	5281794	276.37	$C_{17}H_{24}O_3$	Phenylpropanoid

CID: PubChem Compound Identifier; MW: molecular weight; Da: Dalton.

Results

Molecular docking outcomes: Representative docking results for the priority phytochemical leads against the five metabolic disease targets are summarized in **Table 2**. Binding affinities across all phytochemical-protein pairs ranged from - 6.8 to - 8.4 kcal/mol, consistent with stable and energetically favorable ligand-receptor interactions. All priority compounds matched or exceeded the binding affinity of the positive control, acarbose (- 6.5 kcal/mol against α-glucosidase), thereby validating the docking protocol and supporting the therapeutic plausibility of the identified leads. Nimbolide from *A. indica* was the highest-scoring lead, achieving a docking score of - 8.4 kcal/mol against PPARγ (PDB: 2PRG) through two hydrogen bonds with Ser342 and His323, complemented by van der Waals contacts with Ile341. This binding pattern closely resembles that reported for the thiazolidinedione agonist rosiglitazone within the PPARγ ligand-binding domain. Given the pivotal role of PPARγ in insulin sensitization, adipogenesis, and systemic metabolic regulation, nimbolide represents a promising preclinical candidate for T2DM management.

Table 2: Representative molecular docking scores and binding interactions of prioritized phytochemical leads against metabolic disease target proteins

Plant species	Bioactive compound	Target protein (PDB ID)	Docking score (kcal/mol)	H-bonds (no.)	Other interactions
Moringa oleifera	*Quercetin*	α-Glucosidase (3W37)	- 7.3	Asp349, Arg439 (2)	Hydrophobic: Trp391
Curcuma longa	*Curcumin*	DPP-4 (2I78)	- 7.0	Glu205, Tyr547 (2)	π–π stacking: Phe357
Azadirachta indica	*Nimbolide*	PPARγ (2PRG)	- 8.4	Ser342, His323 (2)	Van der Waals: Ile341
Vernonia amygdalina	*Chlorogenic acid*	α-Amylase (1B2Y)	- 6.8	Asp197, Glu233, Arg195 (3)	-
Hibiscus sabdariffa	*Hibiscetin*	GLUT2 (5EQG)	- 7.6	Gln457, Asn288 (2)	Hydrophobic: Trp420
Zingiber officinale	*6-Gingerol*	α-Glucosidase (3W37)	- 7.0	Asp349, His600 (2)	Hydrophobic: Phe649
Acarbose (reference)	–	α-Glucosidase (3W37)	- 6.5	Asp349, Arg439 (2)	Ionic: Asp408

H-bonds: hydrogen bonds; No.: number of hydrogen bonds identified; PDB: Protein Data Bank; PPARγ: peroxisome proliferator-activated receptor gamma; DPP-4: dipeptidyl peptidase-4; GLUT2: glucose transporter type 2

Hibiscetin from *H. sabdariffa* achieved a docking score of - 7.6 kcal/mol against GLUT2 (PDB: 5EQG), forming hydrogen bonds with Gln457 and Asn288 alongside hydrophobic contacts with Trp420. As GLUT2 is the principal hepatic facilitative glucose transporter regulating postprandial glucose flux, its inhibition may attenuate hyperglycemia. This result is consistent with reports of improved glucose homeostasis in diabetic animal models administered *H. sabdariffa* extracts. Chlorogenic acid from *V. amygdalina* inhibited α-amylase (PDB: 1B2Y) with a docking score of - 6.8 kcal/mol, engaging catalytic residues Asp197, Glu233, and Arg195 through hydrogen bonding. Inhibition of α-amylase delays the hydrolysis of dietary polysaccharides, thereby attenuating postprandial glucose excursions. This observation is consistent with previous reports describing antidiabetic activity among the phenolic and sesquiterpene lactone constituents of *V. amygdalina*, including chlorogenic acid and vernodalin [13], and reinforces the pharmacological rationale underlying the traditional use of this plant in metabolic disease management across West Africa. Quercetin from *M. oleifera* and 6-gingerol from *Z. officinale* exhibited α-glucosidase inhibition with docking scores of - 7.3 and - 7.0 kcal/mol, respectively, both surpassing the positive control acarbose (- 6.5 kcal/mol). Quercetin formed two hydrogen bonds with Asp349 and Arg439, together with hydrophobic interactions at Trp391. 6-Gingerol similarly engaged Asp349 and His600 through hydrogen bonds, with additional hydrophobic contacts at Phe649. These findings align with prior computational and experimental evidence supporting quercetin and 6-gingerol as natural α-glucosidase inhibitors [14, 15]. Curcumin from *C. longa* displayed a docking score of - 7.0 kcal/mol against DPP-4 (PDB: 2I78), engaging catalytic residues Glu205 and Tyr547 through hydrogen bonds and Phe357 through π-π stacking. This finding supports established evidence of curcumin's dual inhibitory activity against DPP-4 and α-glucosidase, further substantiating its relevance as a multi-target antidiabetic phytochemical [16].

ADMET profiles and drug-likeness: ADMET properties of the six priority leads are summarized in **Table 3**. All compounds satisfied Lipinski's Rule of Five, with molecular weights ranging from 294.3 Da (6-gingerol) to 466.5 Da (nimbolide), logP values within acceptable limits, and HBD/HBA counts within the defined thresholds. Oral bioavailability was predicted as moderate to high for all leads using the BOILED-Egg model in SwissADME. Chlorogenic acid, hibiscetin, and quercetin displayed favourable aqueous solubility profiles, a property of particular relevance for formulation into low-cost solid oral dosage forms suited to resource-limited settings. None of the priority leads triggered structural alerts for genotoxicity in AMES mutagenicity prediction, and hepatotoxicity risk was classified as low across all compounds in ADMETlab 3.0 analysis. Nimbolide displayed strong CYP3A4 compatibility, indicating a low probability of clinically significant

metabolic drug-drug interactions. Together, these profiles support the suitability of the identified leads for further preclinical study.

Table 3: ADMET profiles and drug-likeness parameters of prioritized phytochemical leads

Compound	MW (Da)	logP	HBD	HBA	AMES mutagenicity	Hepatotoxicity	CYP3A4 compatibility
Quercetin	302.2	1.54	5	7	Non-mutagenic	Low	Compatible
Curcumin	368.4	3.29	2	6	Non-mutagenic	Low	Compatible
Nimbolide	466.5	3.82	1	7	Non-mutagenic	Low	Compatible
Chlorogenic acid	354.3	- 0.46	6	9	Non-mutagenic	Low	Compatible
Hibiscetin	318.2	0.97	6	8	Non-mutagenic	Low	Compatible
6-Gingerol	294.3	3.85	2	4	Non-mutagenic	Low	Compatible

MW: molecular weight; logP: octanol-water partition coefficient; HBD: hydrogen bond donor; HBA: hydrogen bond acceptor; CYP3A4: cytochrome P450 3A4. All data predicted using SwissADME and ADMETlab 3.0

AI-assisted lead prioritisation: The RF classifier assigned pActive scores ≥ 0.78 to quercetin, nimbolide, hibiscetin, and curcumin, indicating strong probabilistic bioactivity against T2DM-relevant targets and corroborating the docking-based prioritization. AI-assisted screening reduced the computational time and resource burden associated with exhaustive docking of the full phytochemical library, in agreement with the efficiency of machine-learning-based approaches for identifying plant-derived drug candidates [10, 12, 17].

Discussion

Molecular mechanisms and comparative pharmacology: The docking pose of nimbolide within the PPARγ ligand-binding domain, anchored by hydrogen bonds with Ser342 and His323 and reinforced by van der Waals contacts with Ile341, closely resembles the binding mode previously described for the thiazolidinedione agonist rosiglitazone. Given the central role of PPARγ in adipocyte differentiation, insulin sensitization, and systemic lipid handling, this structural similarity suggests that nimbolide may exert insulin-sensitizing activity through a mechanism analogous to synthetic PPARγ agonists, potentially without the fluid retention and cardiovascular liabilities historically associated with thiazolidinediones. This observation is consistent with growing evidence that plant-derived terpenoids can engage nuclear hormone receptors through partial agonism, offering a potentially more favorable safety margin than full synthetic agonists [7]. Similarly, the inhibitory interaction identified between hibiscetin and GLUT2 is mechanistically consistent with earlier pharmacological reports of improved glucose homeostasis in diabetic animal models administered *H. sabdariffa* extracts, and supports a role for anthocyanin- and flavonol-rich *Hibiscus* phytochemicals in attenuating postprandial hyperglycaemia through modulation of hepatic and intestinal glucose transport [3]. The dual-target activity observed for curcumin, engaging DPP-4 and α-glucosidase, corroborates earlier docking and enzymatic-assay evidence for curcumin's multi-target antidiabetic pharmacology [16], and reinforces the therapeutic advantage of polypharmacological phytochemicals over single-target synthetic agents in the management of a multifactorial disease such as T2DM [18].

Clinical and therapeutic implications: From a translational perspective, compounds capable of simultaneously engaging complementary targets, for example, α-glucosidase and α-amylase inhibition to blunt carbohydrate digestion, alongside PPARγ agonism to improve peripheral insulin sensitivity may offer combinatorial glycemic control comparable to, or exceeding, single-mechanism pharmacotherapies, while potentially reducing pill burden and treatment cost within resource-limited health systems. The favorable ADMET and drug-likeness profiles observed for nimbolide, hibiscetin, quercetin, and curcumin support their advancement into in vitro enzymatic and cell-based validation, followed by pharmacokinetic and toxicological evaluation in appropriate animal models, before any consideration of early-phase clinical investigation.

Agricultural relevance and sustainability: The six medicinal plants examined in this study are widely and sustainably cultivated across West Africa, offering a scalable and agronomically integrated source of

phytochemical raw material. Their cultivation requires substantially fewer industrial inputs than synthetic pharmaceutical manufacturing, and their incorporation into agroforestry and crop-improvement policy can concurrently advance food security, biodiversity conservation, and pharmaceutical supply-chain resilience. Nonetheless, climate-induced variability in phytochemical composition represents an emerging challenge to the reproducibility of plant-derived drug discovery, and AI-assisted prediction of metabolite variation under differing agroclimatic conditions constitutes an important avenue for future investigation [19].

AI-driven drug discovery and its significance: The integration of AI-assisted prioritization with molecular docking substantially narrowed the phytochemical search space, directing computational and, by extension, future experimental resources toward the compounds most likely to exhibit genuine bioactivity. This approach is particularly well suited to resource-constrained research environments, where access to high-throughput experimental screening infrastructure remains limited. In the context of Africa's escalating metabolic disease burden and constrained healthcare expenditure, such AI-enabled computational pipelines provide a cost-effective, high-throughput mechanism for generating and prioritizing preclinical drug candidates, thereby expanding equitable research capacity in low-resource settings. This approach aligns with Sustainable Development Goal 3 (Good Health and Well-Being) and supports the development of African-led pharmaceutical innovation [8, 9].

Limitations: Molecular docking provides a static, rigid or semi-flexible approximation of ligand-receptor binding and does not fully capture the dynamic conformational behavior, solvation effects, or entropic contributions that govern binding within a physiological environment; docking scores should therefore be interpreted as indicative rather than definitive measures of binding affinity. The RF prioritization model, although demonstrating good cross-validated performance, was trained on bioactivity data that may not fully represent the structural chemical space occupied by the phytochemicals examined here. Also, no in vitro enzymatic, cell-based, or in vivo validation was undertaken in the present study, and the ADMET predictions, while informative for early triage, require confirmation through experimental pharmacokinetic assays.

Future direction: Future work should prioritize *in vitro* enzyme inhibition assays and cell-based glucose uptake studies to validate the docking-predicted activities of nimbolide, hibiscetin, quercetin, and curcumin, followed by molecular dynamics simulations to assess the stability of the predicted binding poses over physiologically relevant timescales. Parallel efforts should focus on developing curated, Africa-specific phytochemical and bioactivity databases to improve the training data for AI-assisted prioritization models, alongside agroclimatic studies exploring how cultivation conditions influence phytochemical yield and composition in these species.

Conclusion: The strategic integration of ethnopharmacological knowledge, molecular docking, ADMET profiling, and AI-assisted lead prioritization constitutes a scientifically rigorous and resource-efficient framework for phytochemical drug discovery. Nimbolide, hibiscetin, quercetin, and curcumin, all sourced from commonly cultivated agricultural species, exhibited binding affinities comparable to or exceeding that of the reference drug acarbose against validated metabolic disease targets, alongside favorable ADMET profiles and drug-likeness parameters supporting their preclinical advancement.

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